



ADMET Group Leaderboard

- TDC.Caco2_Wang

Leaderboard
- TDC.Bioavailability_Ma

Leaderboard
- TDC.Lipophilicity_AstraZeneca

Leaderboard
- TDC.Solubility_AqSolDB

Leaderboard
- TDC.HIA_Hou

Leaderboard
- TDC.Pgp_Broccatelli

Leaderboard
- TDC.BBB_Martins

Leaderboard
- TDC.PPBR_AZ

Leaderboard
- TDC.VDss_Lombardo

Leaderboard
- TDC.CYP2C9_Veith

Leaderboard
- TDC.CYP2D6_Veith

Leaderboard
- TDC.CYP3A4_Veith

Leaderboard
- TDC.CYP2C9_Substrate_CarbonMangels

Leaderboard
- TDC.CYP2D6_Substrate_CarbonMangels

Leaderboard
- TDC.CYP3A4_Substrate_CarbonMangels

Leaderboard
- TDC.Half_Life_Obach

Leaderboard
- TDC.Clearance_Hepatocyte_AZ

Leaderboard
- TDC.Clearance_Microsome_AZ

Leaderboard
- TDC.LD50_Zhu

Leaderboard
- TDC.hERG

Leaderboard
- TDC.AMES

Leaderboard
- TDC.DILI

Leaderboard

References

- Submission Instructions
- BenchmarkGroup Class Documentation
- Leaderboard Guidelines

TDC.Solubility_AqSolDB

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Dataset Summary

Dataset	Unit	Size	Task	Metric	Dataset Split
TDC.Solubility_AqSolDB	log mol/L	9,982	Regression	MAE	Scaffold

Leaderboard

↕ for history. Search history with c-↕/c-↓

Rank	Model	Contact	Link	#Params	MAE ↓
1	Chemprop-RDKit	Kyle Swanson	GitHub, Paper	N/A	0.761 ± 0.025
2	AttentiveFP	Kexin Huang	GitHub, Paper	300,806	0.776 ± 0.008
3	MapLight + GNN	Jim Notwell	GitHub, Paper	N/A	0.789 ± 0.003
4	MapLight	Jim Notwell	GitHub, Paper	N/A	0.792 ± 0.002
5	RDKit2D + MLP (DeepPurpose)	Kexin Huang	GitHub, Paper	633,409	0.827 ± 0.047
6	Basic ML	Nilavo Boral	GitHub, Paper	N/A	0.828 ± 0.002
7	Chemprop	Kyle Swanson	GitHub, Paper	N/A	0.829 ± 0.022
8	GCN	Kexin Huang	GitHub, Paper	191,810	0.907 ± 0.020
9	CFA	Nan Jiang	GitHub, Paper	N/A	0.939 ± 0.030
10	NeuralFP	Kexin Huang	GitHub, Paper	480,193	0.947 ± 0.016
11	CNN (DeepPurpose)	Kexin Huang	GitHub, Paper	226,625	1.023 ± 0.023
12	AttrMasking	Kexin Huang	GitHub, Paper	2,067,053	1.026 ± 0.020
13	ContextPred	Kexin Huang	GitHub, Paper	2,067,053	1.040 ± 0.045
14	Euclia ML model	Euclia	GitHub, Paper	50	1.076 ± 0.016
15	Morgan + MLP (DeepPurpose)	Kexin Huang	GitHub, Paper	1,477,185	1.203 ± 0.019

↓: The lower the better.